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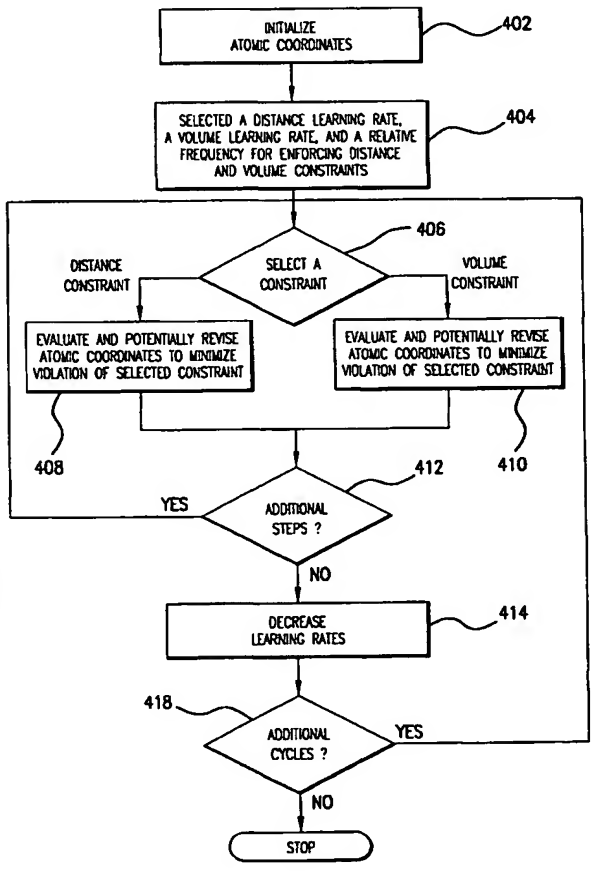
(54) Title: CONFORMATIONAL SAMPLING BY SELF-ORGANIZATION



(57) Abstract: A self-organizing method, system, and computer program product for generating molecular conformations that are consistent with a set of distance and/or volume constraints. A stochastic proximity embedding (SPE) algorithm evaluates individual distance and/or volume constraints and adjusts the atomic coordinates to minimize violations of such constraints. The method scales linearly with thenumber of atoms, and produces many more unique conformations at a fraction of the time required by conventional distance geometry algorithms.

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